

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060623\
 Data File : BG057646.D
 Acq On : 6 Jun 2023 20:58
 Operator : CG/JU
 Sample : 02997-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DMA-1105

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.857	389	395	409	rBV	172884	300651	13.90%	3.854%
2	7.490	667	673	686	rBV	111565	209767	9.70%	2.689%
3	8.336	810	817	826	rBV	73787	125187	5.79%	1.605%
4	9.523	1011	1019	1033	rBV	277210	514408	23.79%	6.593%
5	11.180	1293	1301	1308	rBV	105088	193200	8.94%	2.476%
6	11.667	1378	1384	1389	rBV	14441	24430	1.13%	0.313%
7	13.582	1702	1710	1719	rBV	892646	1409836	65.20%	18.070%
8	14.957	1937	1944	1951	rBV	199917	308025	14.25%	3.948%
9	16.290	2165	2171	2178	rBV	37944	56524	2.61%	0.724%
10	16.443	2190	2197	2209	rBV	704914	1129953	52.26%	14.483%
11	17.694	2404	2410	2419	rVB	271068	402541	18.62%	5.160%
12	18.534	2548	2553	2558	rBV2	38420	59960	2.77%	0.769%
13	20.261	2841	2847	2853	rBV	1637955	2162222	100.00%	27.714%
14	21.565	3064	3069	3079	rBV5	28225	77366	3.58%	0.992%
15	22.000	3136	3143	3152	rVB	242333	416696	19.27%	5.341%
16	25.490	3728	3737	3748	rVB	141672	411104	19.01%	5.269%

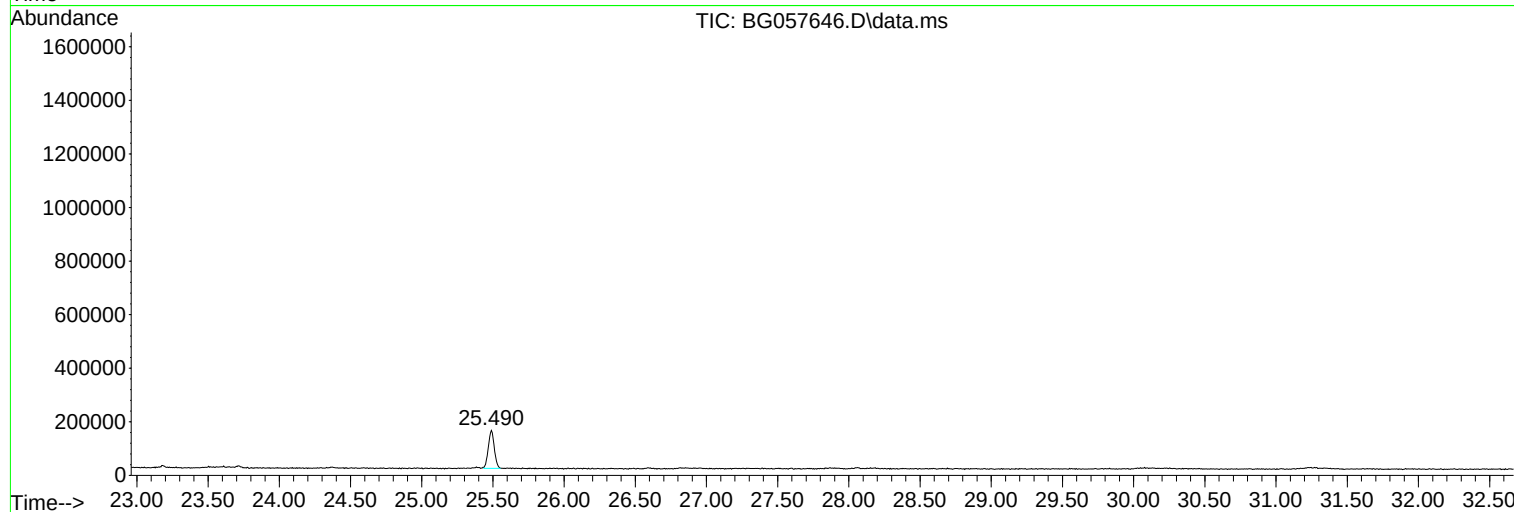
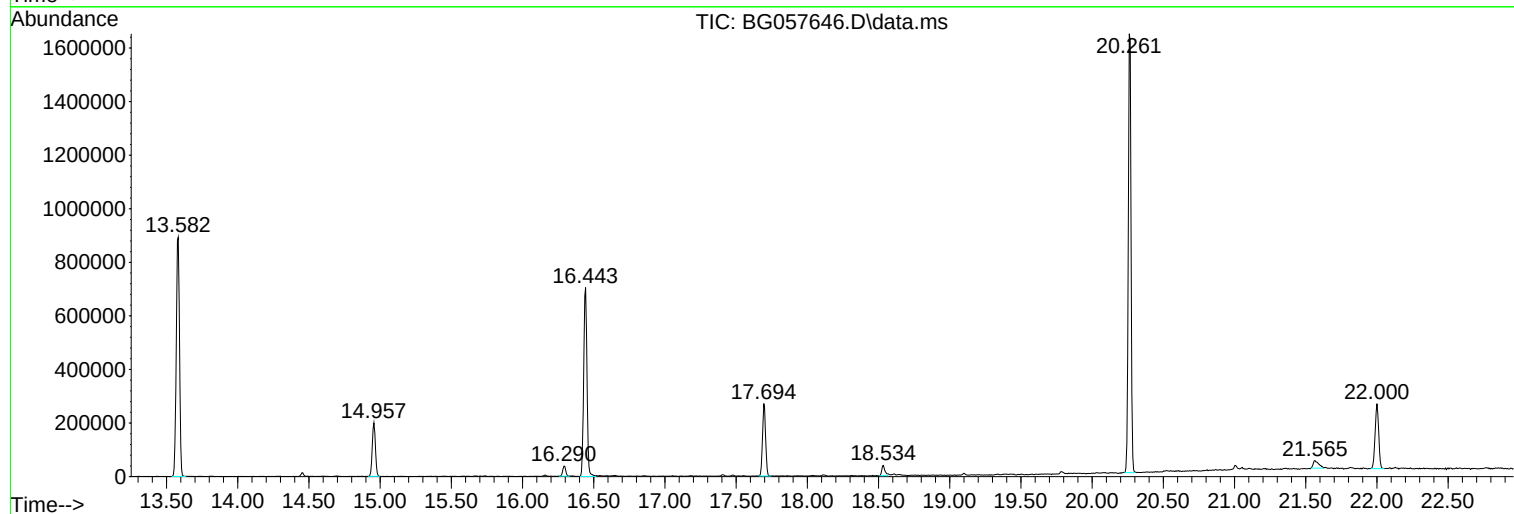
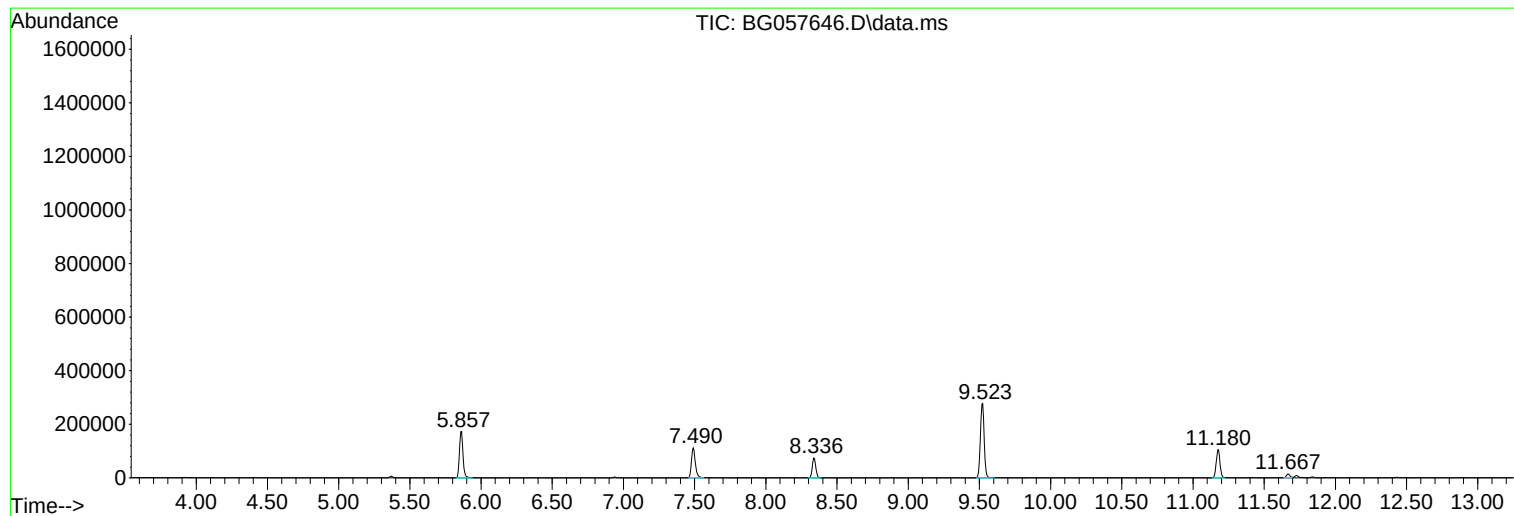
Sum of corrected areas: 7801870

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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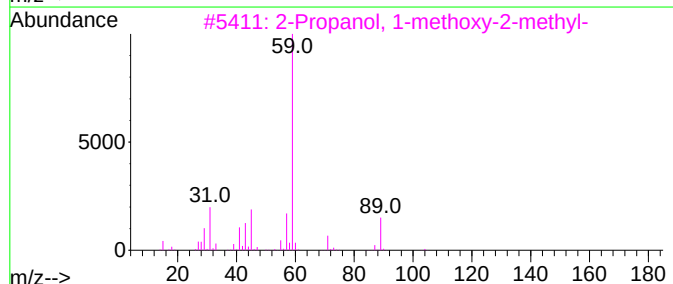
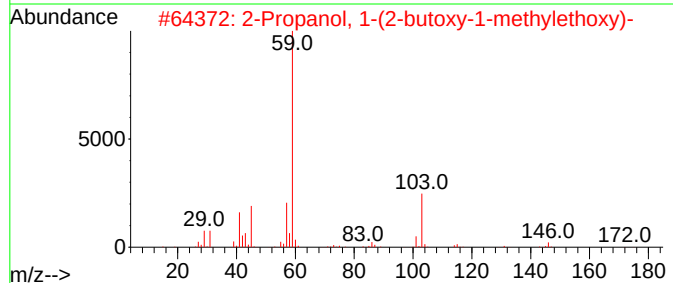
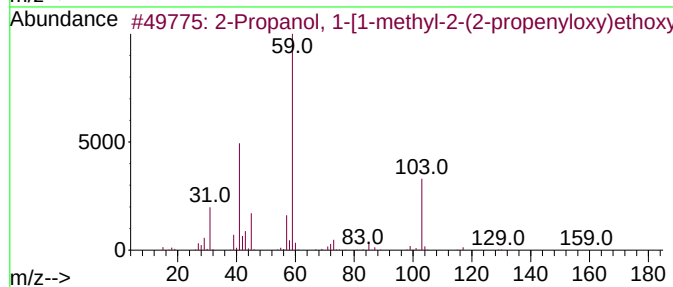
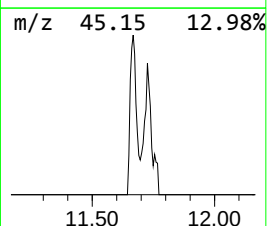
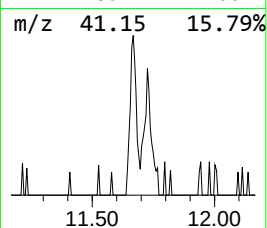
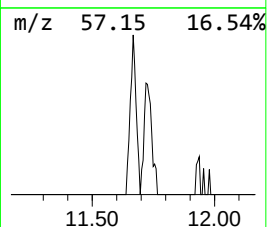
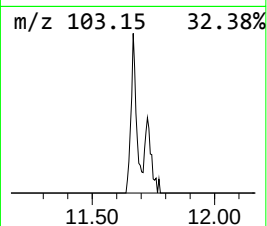
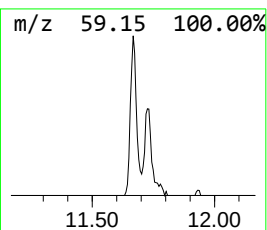
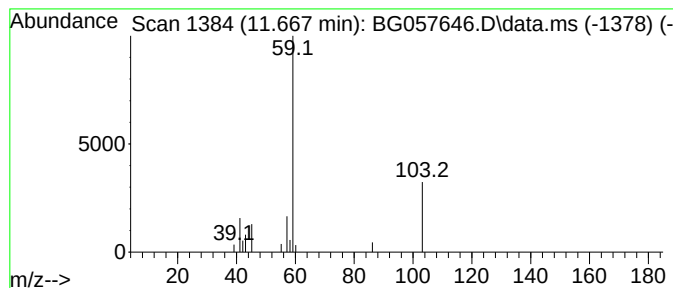
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.667	2.53 ng	24430	Naphthalene-d8	11.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78		
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74		
3	2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	50		
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	40		
5	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	39		



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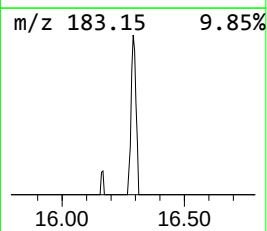
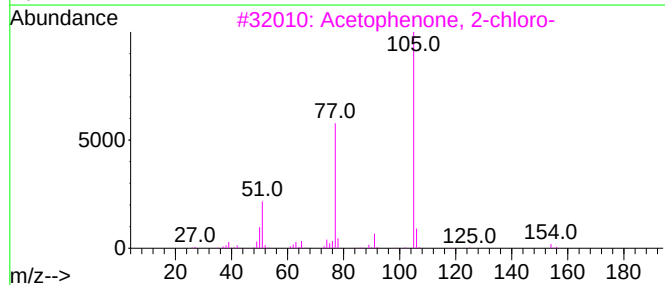
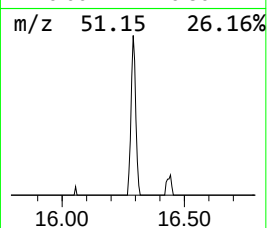
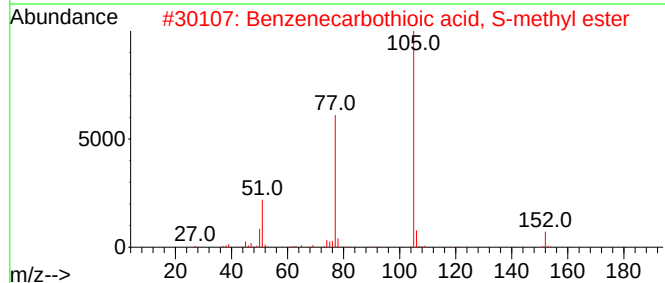
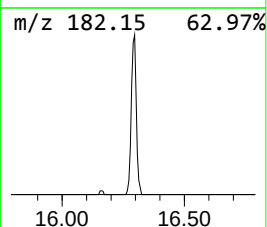
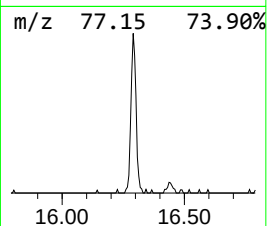
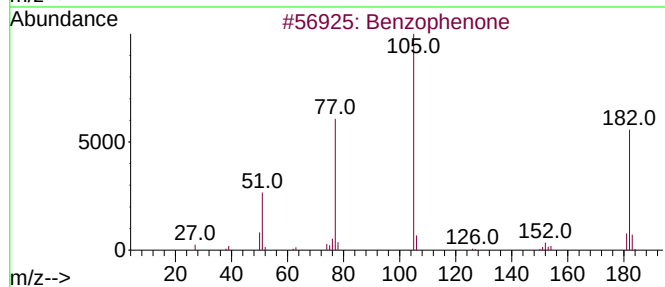
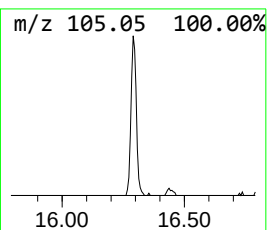
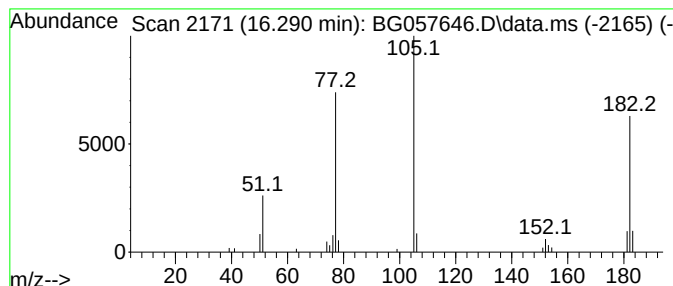
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.290	3.67 ng	56524	Acenaphthene-d10	14.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	50



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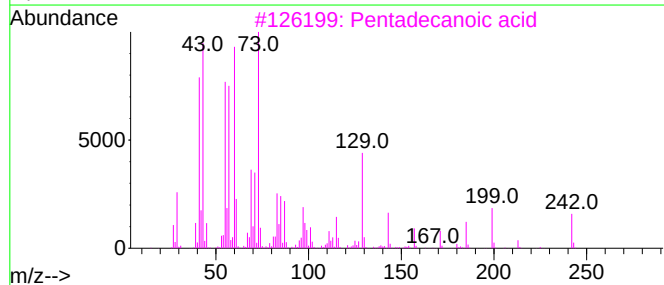
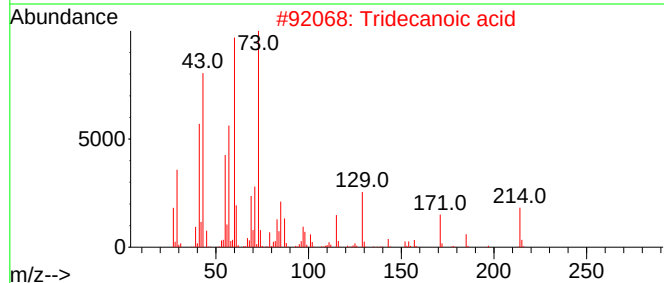
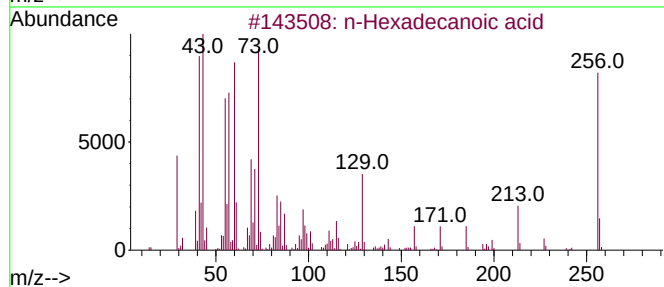
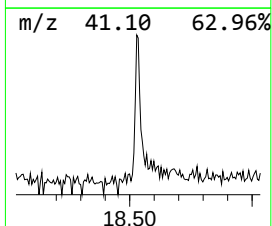
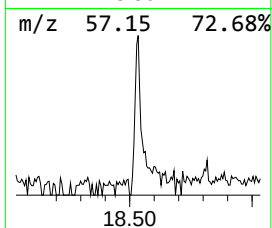
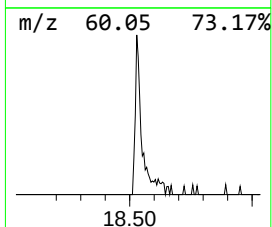
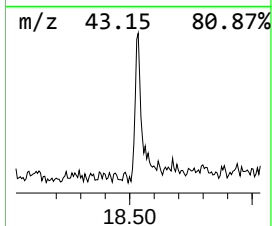
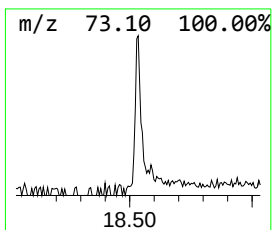
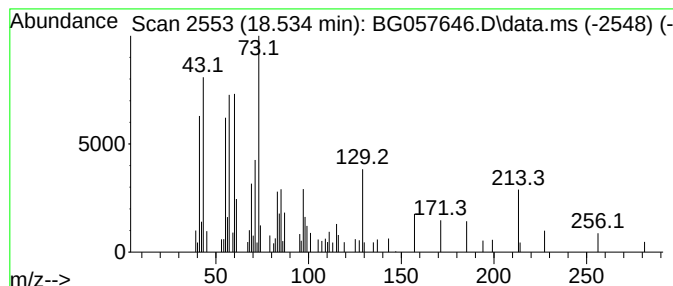
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.534	2.98 ng	59960	Phenanthrene-d10	17.694

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	62
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			Sulfurous acid, 2-propyl tetra...	320	C17H36O3S	1010309-12-5	18



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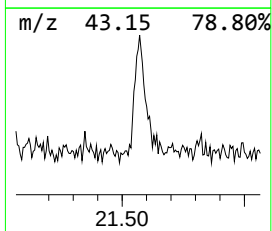
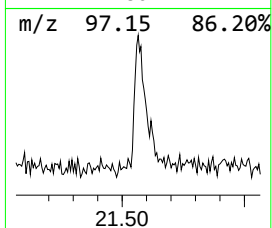
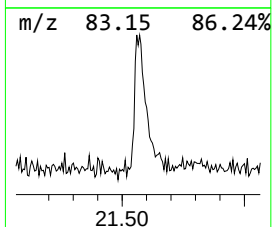
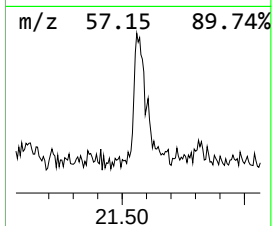
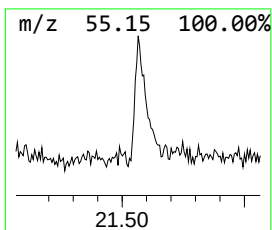
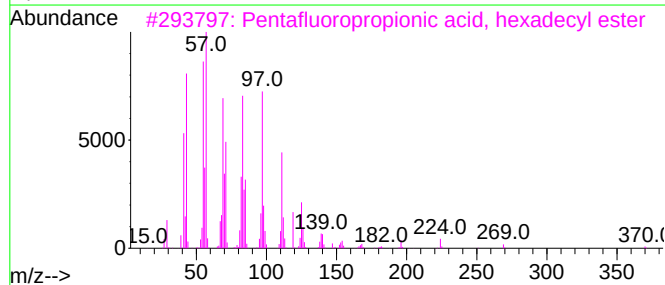
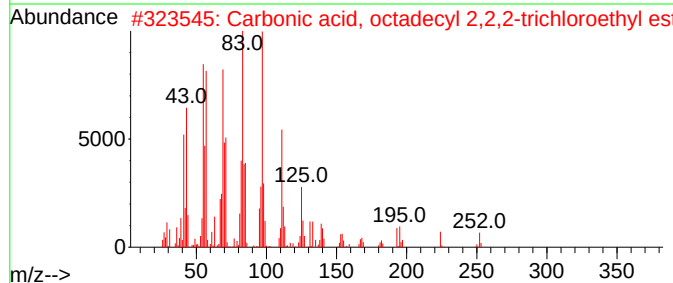
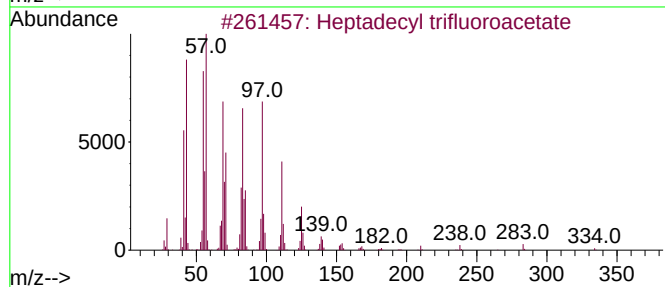
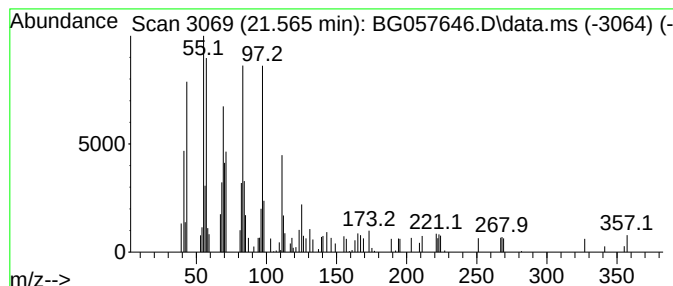
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Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.565	3.71 ng	77366	Chrysene-d12	22.000

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
2			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 1-[...]	11.667	2.5	ng	24430	2	11.180	193200	20.0
Benzophenone	16.290	3.7	ng	56524	3	14.957	308025	20.0
n-Hexadecanoic ...	18.534	3.0	ng	59960	4	17.694	402541	20.0
Heptadecyl trif...	21.565	3.7	ng	77366	5	22.000	416696	20.0